

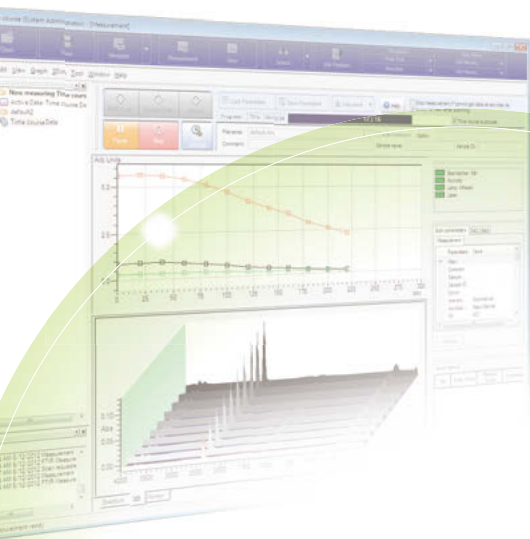
Analytical Data System for FTIR

LabSolutions IR



Next-Generation Workstation Designed for the Future

Network-enabled as part of the LabSolutions family, LabSolutions IR is furnished with rich spectral libraries and a high-performance search function as standard. Labor-saving macros provide for a higher level of automation and improved work efficiency.



Network-Enabled

**Rich Libraries and
a High-Performance
Search Function**

LabSolutions IR

**Macro Functions Provide
Automation and Labor-Savings**



Three Major Advantages of LabSolutions IR

Network-Enabled

P. 4

- As a part of the LabSolutions family of control software, LabSolutions IR provides advanced security and user administration features.
- Complies with ER/ES regulations including FDA 21 CFR Part 11 and PIC/S.
- Centralized management of valuable FTIR data, as well as LC and GC data, on a networked server allows simple control over security and backups.
- Terminal Services can be used to control LabSolutions IR from a remote location, even when LabSolutions IR is not installed on the client PC.

Rich Libraries and a High-Performance Search Function

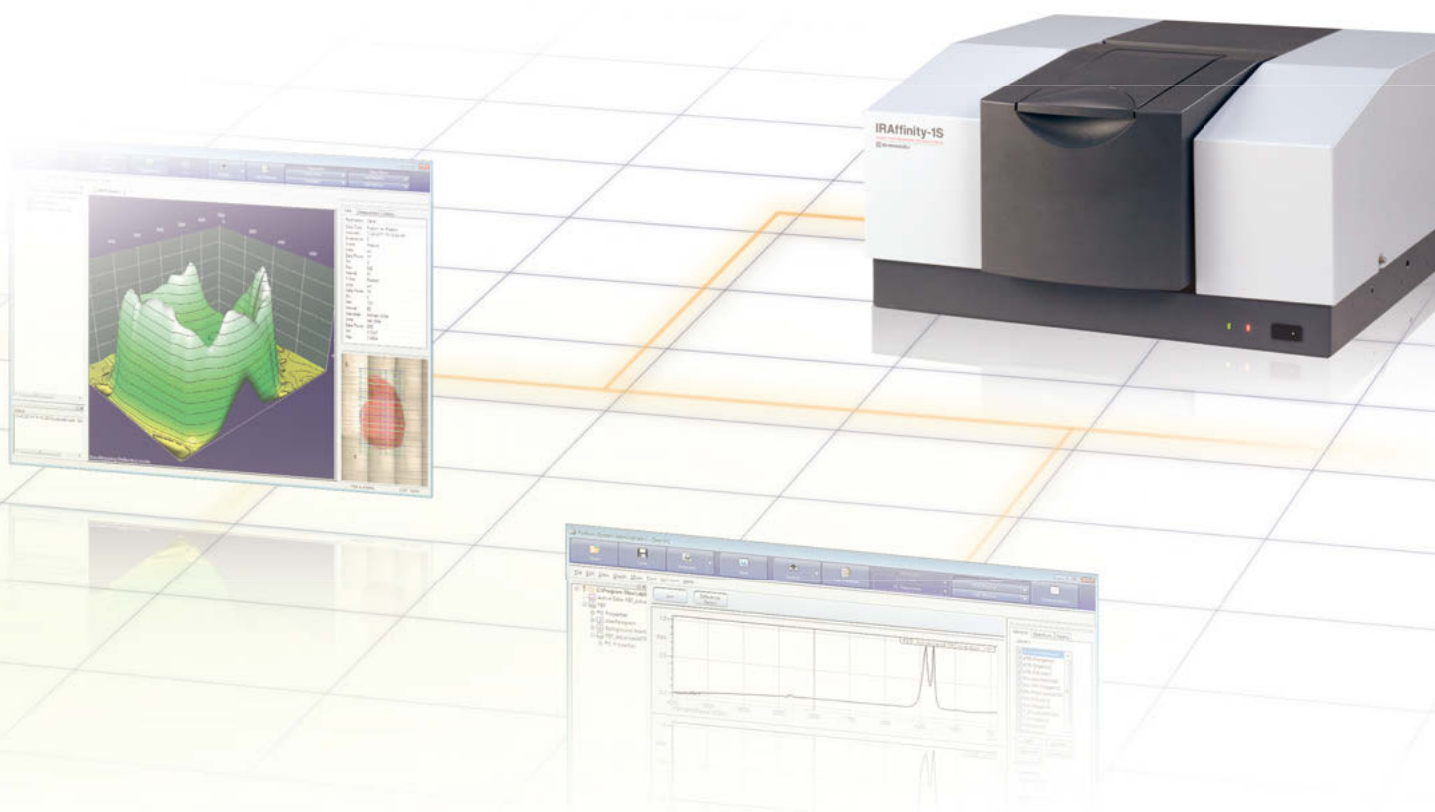
P. 8

- A library of approximately 12,000 spectra included as standard
- The standard library alone has enough data to furnish productive searching.
- Advanced library search functions include spectral search, text search, compound search, and peak search.
- Employing Shimadzu's unique search algorithms for a high hit rate.

Macro Functions Provide Automation and Labor-Savings

P. 10

- A simple macro function allows the user to execute multiple operations by simply creating a list of operational steps.
- Contaminant analysis and identification tests are automatically done through use of macros for a more efficient workflow.



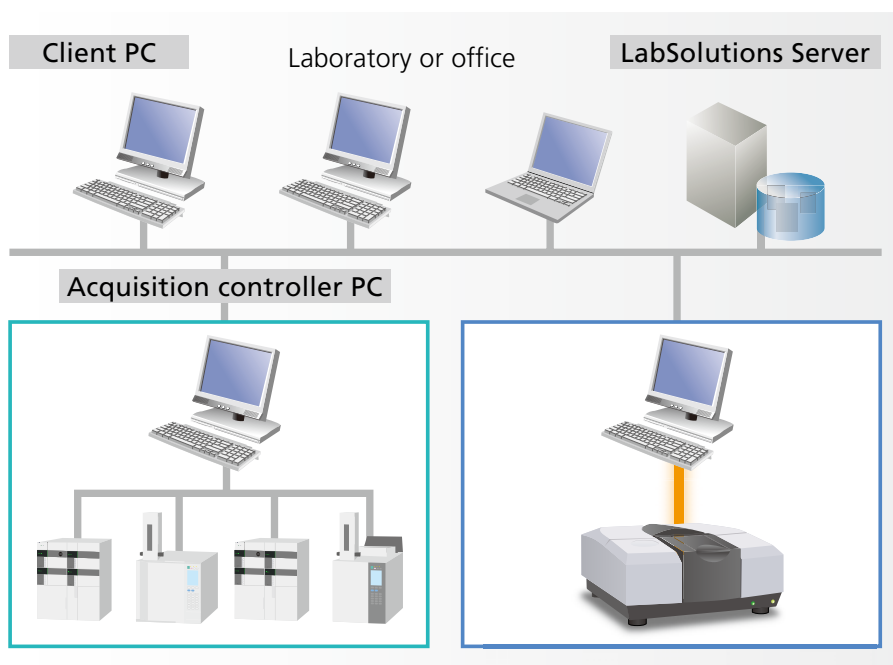
Creating an Integrated Laboratory Network

Manage your valuable data from a centralized networked server. The LabSolutions IR Series enables networked management of FTIR as well as LC and GC data. In addition, it is capable of managing a wide variety of analytical instruments on a network.

◆ LabSolutions CS

When connected without restrictions to an analytical network, LabSolutions CS manages all analytical data in a central database on a server computer, facilitating access to analytical data from any computer connected to that network. Terminal Services (RemoteApp) can also be used to control LabSolutions IR from a remote location, even

when LabSolutions IR is not installed on the client PC. LabSolutions CS is ideal for customers wanting compliance with ER/ES regulations while seeking to manage LC/GC data together with FTIR data on one server hosting a large number of users.



Name	LabSolutions IR	LabSolutions DB IR	LabSolutions CS
Data management method	Measured data files are saved and managed in folders on the PC.	Measured data files are saved and managed in the LabSolutions database.	
Data references	The software references files on drives or in folders on the PC.	The software references files in the database.	
LabSolutions database	Unavailable	Available (The database resides on a local PC)	Available (The database resides on a server)
CLASS-Agent database	Available (Option)	Unavailable (The contents of the CLASS-Agent database can be transferred to the LabSolutions database.)	
User administration		Available	
Rights group administration		Available	
Project administration	Unavailable	Available	
Standalone/network	Either can be used.	Only the standalone configuration can be used.	Only databases on the network can be used. (LabSolutions IR data can be viewed using the database manager on a PC set up for viewing purposes. Note that LabSolutions IR must be installed on the PC used for viewing.)
Data backup	Performed on a file-by-file basis using Windows Explorer.	Performed for each database.	

◆ LabSolutions DB IR

LabSolutions DB IR combines analytical data management functions with LabSolutions IR and is capable of providing secure data management from a single computer. Compliant with FDA 21 CFR Part 11 and PIC/S, LabSolutions DB IR is the optimal setup for customers

wanting to manage all their data from a single computer. It requires no network connection and is recommended for customers who seek ER/ES compliance in a standalone format.



◆ LabSolutions IR

LabSolutions IR is a consolidation of the advanced features found in Shimadzu's earlier IRsolution control software. In addition to improved operability, LabSolutions IR employs advanced management functions to provide a safe and highly reliable system solution.

LabSolutions IR can also be connected to existing CLASS-Agent systems and is therefore recommended for customers who want to use their established methods, or for systems that see a low frequency of use.



Solutions Delivered by the LabSolutions IR Series

LabSolutions IR resolves a number of problems commonly faced in the laboratory.

Provides a superb operating environment.

- The operational status of all instruments on the network can be checked at a glance.
- Analysis can be managed from any computer, not only specialized analytical PCs.
- Quick searches of large volumes of data

Designed to increase efficiency in the performance of management tasks.

- Not only all data, but all system user information is managed centrally on a server.
- Information management on a project-by-project basis

Delivers safe and reliable data management.

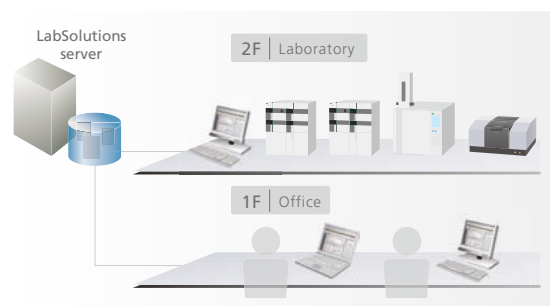
- Prevents mistakes in database management.
- Firm security

Provides total, regulatory-compliant support.

- Assistive features for the execution of CSV activities (IQ/OQ validation, etc.).
- Terminal service does not require LabSolutions software configuration control on client PCs.

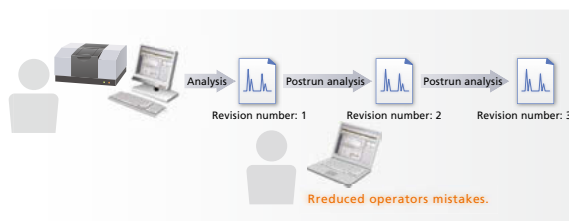
◆ Analyze data from any computer

LabSolutions CS control software allows access to the analytical instruments on the network freely and independent of location while maintaining security. For example, pre-analysis operations can be performed from a computer terminal within the analytical laboratory. After the analytical run is initiated, the operating conditions can then be followed and data analysis performed from a computer located outside the laboratory. This operational format increases efficiency during analytical activities such as progress checks and report writing.



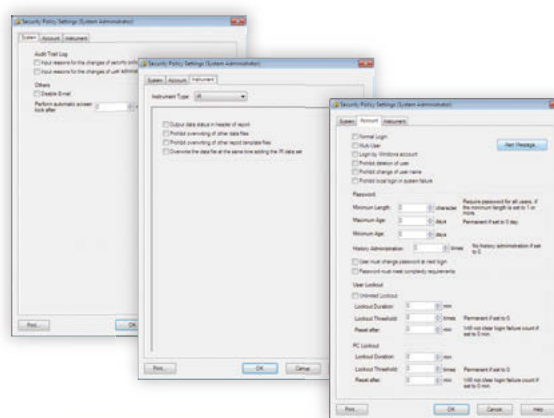
◆ Prevents mistakes in database management.

LabSolutions DB and LabSolutions CS employ a database that ensures the secure management of analytical data. When used for the management of analytical data, this database prevents such mistakes as overwritten or deleted analytical data. This database also manages postrun analyses of analytical data by automatically attributing revision/version numbers to separate analyses, so analytical data is not overwritten. Old data can also be viewed with ease.



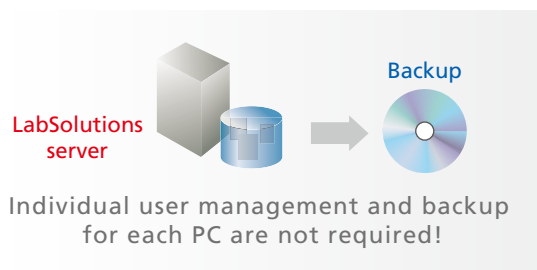
◆ Firm security

Functions for setting an audit trail to ensure data reliability and for e-mailing events occurring on the system can be set. Various settings, such as setting the length, expiration date and complexity of passwords for user accounts, setting the lockout function to prevent illegal access, and registering settings for the deletion and alteration of registered users, can be made to enable highly secure system operation. Settings for overwriting data files and other information and settings relating to items to output in reports are also supported.



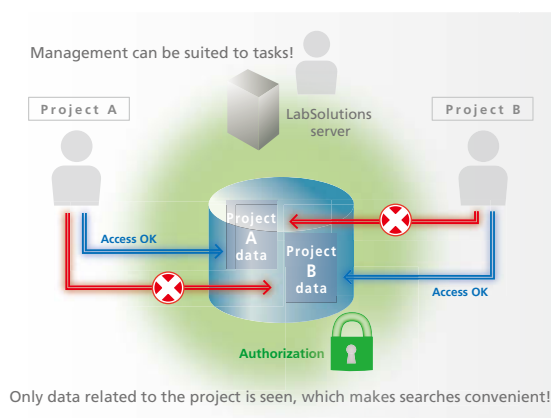
◆ In addition to data, all user and other system information is managed centrally on a server.

In situations where user information is managed on each individual computer terminal, increasing the number of computers increases the burden on the person responsible for managing the information. With LabSolutions CS, all user information is managed centrally on the server, reducing the burden of individual computer terminal management and making the terminal administrator's job easier. Backing up data is also important. Because LabSolutions CS manages all data centrally on a server, no data is kept on networked computer terminals. The data stored centrally on the server can be backed up onto DVDs or other storage media, allowing this data to be referenced directly and eliminating the need to carry out a complete restore process.



◆ Information management on a project-by-project basis

LabSolutions DB and LabSolutions CS are designed with project management functions that allow data to be managed for each task or system application. These functions include the ability to configure equipment control, user administration, security policy, and other data processing settings on a project-specific basis, making data search and operational management activities smoother between projects.



◆ Total, regulation-compliant support: Document preparation assistance

Building a system requires the documented formulation of management and operational management procedures, and that the system be operated according to those procedures. The service and work provided by Shimadzu for its customers goes beyond that normally expected of a supplier. Shimadzu assists in the preparation of documents necessitated by various industry regulations, and provides total, comprehensive support over the entire lifecycle of its systems. This begins with

deliberations conducted prior to the installation of a system, and stretches to inspections that follow system installation as well as system updates. Shimadzu also reacts quickly to domestic and foreign trends in new requirements of regulatory authorities and the like. Shimadzu has a complete system of support in a state of continued readiness to meet the demands of its customers.

Sample Architectural Documentation	
[System Developmental Documents]	[System Operational Management Documents]
Validation Plans	Operational Management Standards
Definition of User Requests	Documentation Management Procedures
Supplier Assessment Plans and Reports	Configuration Management and Change Management Procedures
Functional Specifications	System Management Procedures
Configuration Establishment Specifications	Security Management Procedures
DQ Plans and Reports	Backup and Recovery Procedures
IQ/OQ/PQ Plans and Reports	Archiving Procedures
Validation Reports, etc.	Troubleshooting Procedures
	Education and Training Implementation Procedures etc.

Rich Libraries and a High-Performance Search Function

Approximately 12,000 spectra are included as standard with LabSolutions IR. Highly effective searching can be done with standard libraries.

◆ Approximately 12,000-spectra library

A wide variety of libraries, including unique SHIMADZU libraries, reagents, polymers, and more are included as standard. Searching with standard libraries provides high-quality results without purchasing extra libraries.

Contents

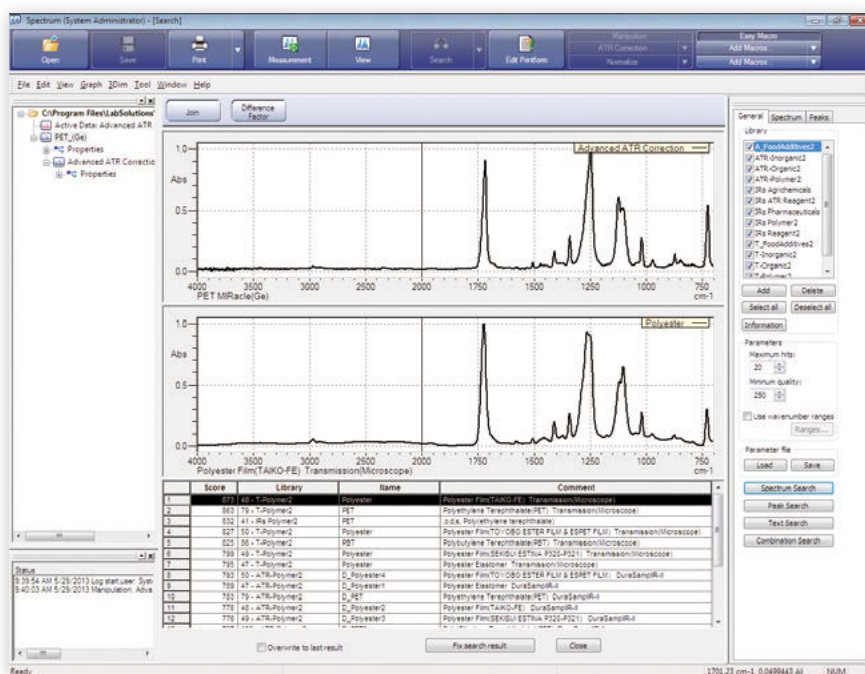
- SHIMADZU Food additives library
 - SHIMADZU Contaminants library
 - Reagents
 - Polymers
 - Pharmaceutical products, agrichemicals
 - Inorganic compounds, etc.
- Total approx. 12,000 spectra

◆ High-performance search functions

LabSolutions IR delivers high-quality of search results with 4 high-performance search methods (spectral search, peak search, text search and combination search) and libraries containing approximately 12,000 spectra. Libraries created on IRsolution and HYPER-IR and commercial libraries such as Sadtler and S.T. Japan can also be used. Simply drag spectra into a library to create a user library. Editing spectrum information or deleting a spectrum in a library is also very easy.

Search functions

- Spectral search
Shimadzu's unique search algorithm provide highly precise results.
- Peak search
If you only have an old spectrum chart, searching can be done with peak wavenumbers without a spectrum file.



◆ Contaminant analysis program

By combining Shimadzu's own algorithms (patent pending) with that of library spectra for common contaminants, this program identifies contaminants with a high degree of accuracy. Reports are automatically created after analysis, thereby reducing post-processing time to a few seconds.

With automated reporting, this easy-to-use program allows operators with little FTIR knowledge to perform analysis easily.

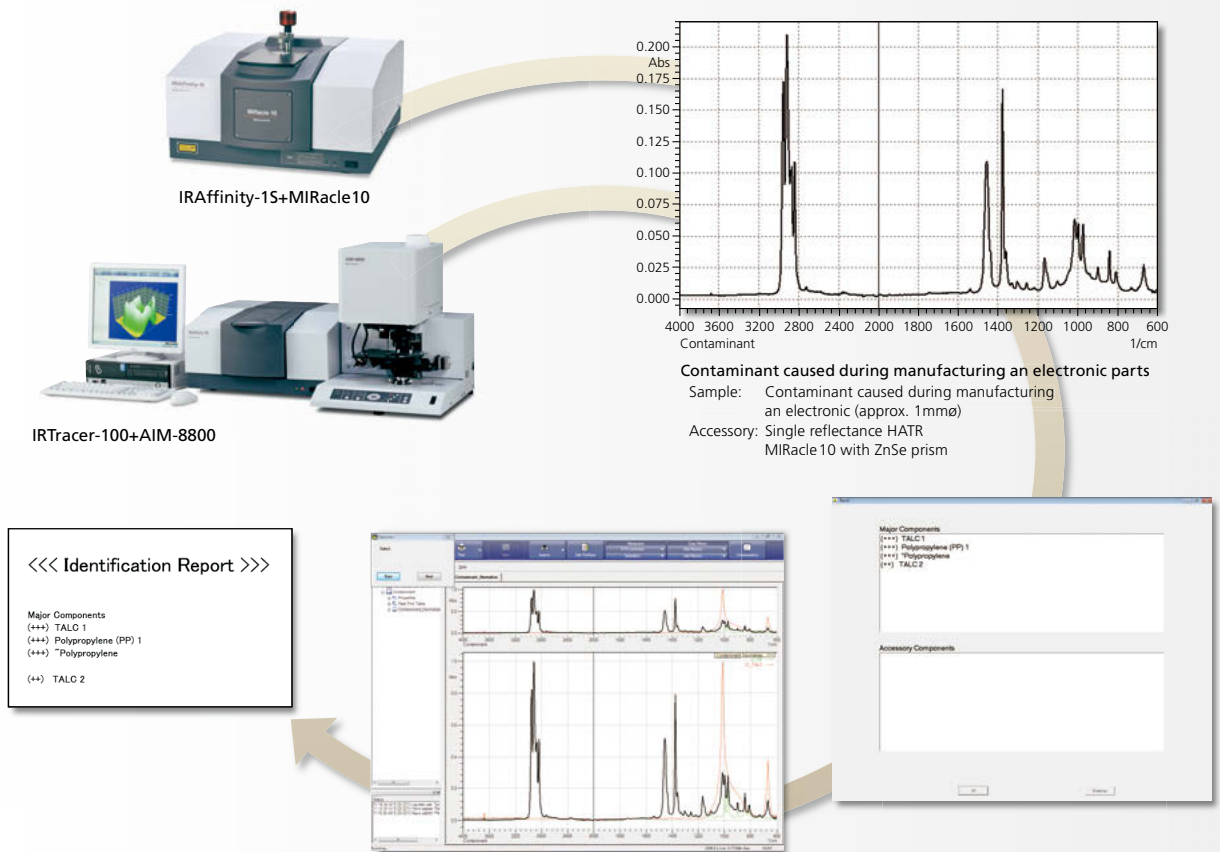
4 features of the Contaminant analysis program

Contains spectra for over 550 highly-selected inorganic substances, organic substances, and polymers that are often detected as contaminants in Shimadzu's Analytical Applications Department.

Allows automation of the process, including searching, judgment evaluation, and report creation.

Incorporates algorithms that focus on spectral characteristics, rather than performing simple spectrum searches.

Major and Minor components are found and their ranks are displayed.



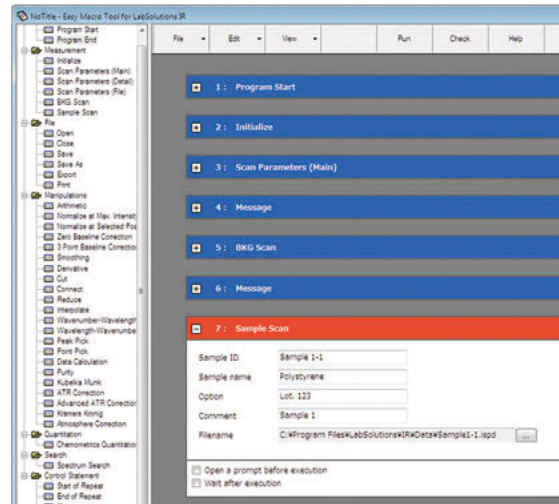
Macro Functions Provide Automation and Labor-Savings

LabSolutions IR automates routine work, such as scanning-data manipulation-reporting, identification tests, and contaminants analysis.

Programs are launched from Launcher or your Desktop.

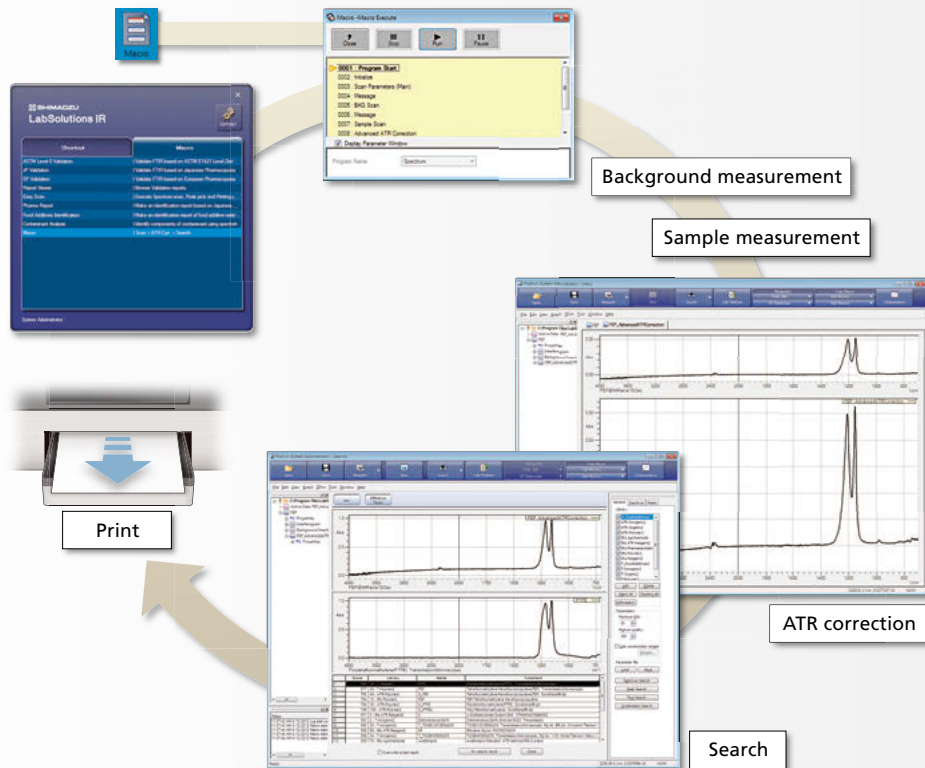
◆ Easy Macro – Just a single click launches routine work.

The “Easy Macro” function will create macros that are suitable for routine work, particularly when repetitive operations are used. The macro builder allows macros to be constructed by simply selecting and aligning operations from a list. Once constructed, the macros can be registered with the Launcher and Desktop for quick execution. Operators not familiar with IR instruments can operate them easily without any mistakes.



Easy Macro Operations

- ▶ Initialization of FTIR, configuration of scan parameters, spectrum measurement
- ▶ Data manipulations, Search, Quantitation, Printing
- ▶ Repeat measurements, Displaying messages, alarm sounds, External program execution



The use of macro programs means automation and labor-saving improvements in the execution of the following analytical work.

- **Routine tasks consisting of measurements, peak detection, and printing**
 - Common, routine tasks for IR analysis can be performed with a single click.
- **Japanese Pharmacopoeia and food additive identification tests**
 - Automatic pass/fail testing of inspection samples
- **Contaminant Analysis**
 - Easy and quick contaminant analysis. Analysis results are provided in Only a few seconds.
- **Validation program that complies with the Japanese, European, Chinese, and United States Pharmacopoeias, and with ASTM**
 - Easy undertaking of instrument inspections in accordance with official regulations

◆ Identification test program

This program makes pass/fail judgments about samples in accordance with the tests specified in the Pharmacopoeia. In addition to identification tests for pharmaceutical products, this program can be used for incoming inspections and pre-shipment inspections.

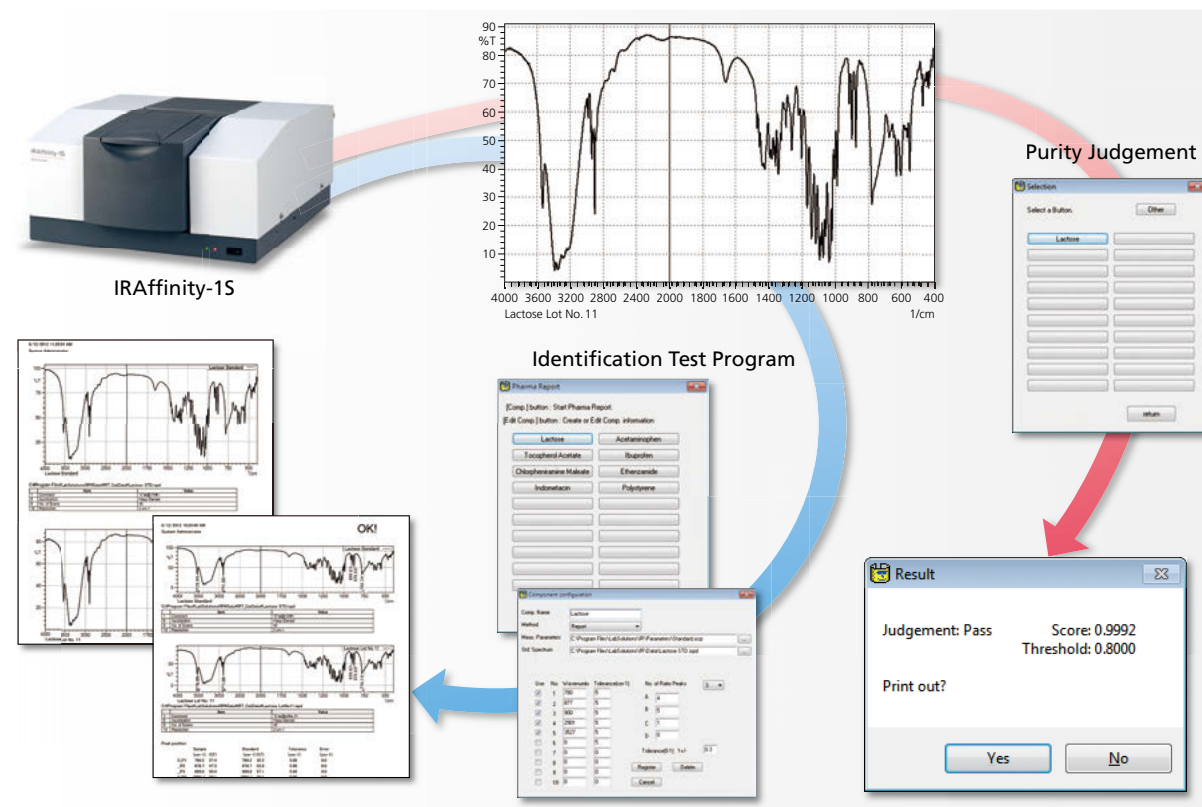
4 features of the Identification test program

Prints out the spectra for standards and samples in order to facilitate easy comparison.

Calculation of the differences between the peak wavenumbers for standards and samples, differences in intensity ratios between peaks, pass/fail judgments, and print out of reports.

Detection and printing just the peaks that are specified for pass/fail judgment.

Spectra of 57 samples on Japanese Standards of Food Additives are stored in LabSolutions IR.



Purity Judgment

The Purity Judge calculates the similarity (Purity) between a reference spectrum and a test spectrum, and judges Pass or Fail. It judges similarity of spectra in a quantitative way.

Software Options

LabSolutions IR incorporates data processing functions such as Advanced ATR correction and Kubelka-Munk conversion, quantitation functions such as the multi-point calibration curve method and the CLS method, as well as the spectral searching function as standard features. However, adding the following optional software products makes it possible to further increase the application range.

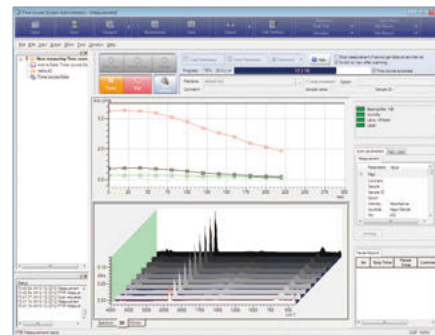
LabSolutions IR

Time course software

(P/N 206-74558-91)

The time course program is used to collect spectra in regular intervals and creates a time course dataset used to follow reactions as a function of time. Changes in peak height and peak area can be used to calculate values related to reaction kinetics. Time course information is saved and displayed in 3D (bird's eye view) or in a contour plot. It can be recalculated by modifying parameters.

The scan interval is dependent on resolution, number of scans and mirror speed. The fastest speed under a 16cm^{-1} resolution and a mirror speed of 9mm/s is 7 seconds for 1 accumulated scan. Maximum measurement time is 48 hours but it depends on scan parameters. The time course software includes a 3D Processing program.



LabSolutions IR

Mapping program

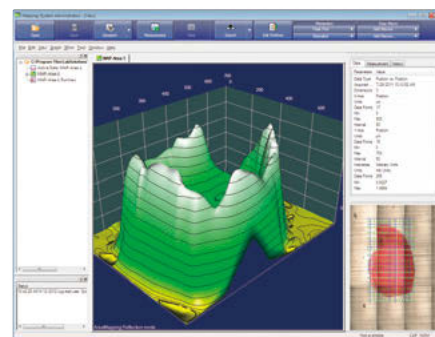
(P/N 206-74559-91)

The Mapping software allows one to map absorption information on a sample surface as a function of position when using the Shimadzu AIM-8800 Infrared Microscope.

Mapping parameters, such as the mapping range, the scan intervals, and the background positions, can be set on the composite images. Area mapping, line mapping and random mapping modes are supported.

In addition to mapping in the conventional transmittance and reflectance modes, micro-ATR mapping with an optional ATR objective is also available. From the acquired mapping data, it is possible to extract spectra and to perform calculations for functional-group mappings for specific peaks. The data can be displayed as 3D images or contour plots, or in spectral overlay mode.

Mapping program includes a 3D Processing program.



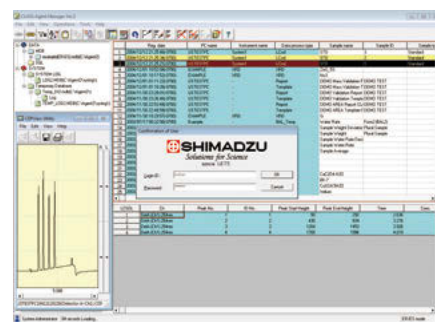
CLASS-Agent connection kit

(P/N 206-74557-91)

This is a program to connect LabSolutions IR (File edition) to the CLASS-Agent system. Spectra collected using LabSolutions IR are managed in an existing CLASS-Agent database. The database enables data management for the entire recording life cycle, which consists of the creation (measurement), inspection, approval, storage, browsing, backup, and disposal of analysis data.

CLASS-Agent Manager and Public Agent are required.

* Only spectra are saved in the CLASS-Agent database. Mapping data, Time course data, Calibration curve and Quantitation result tables cannot be stored.

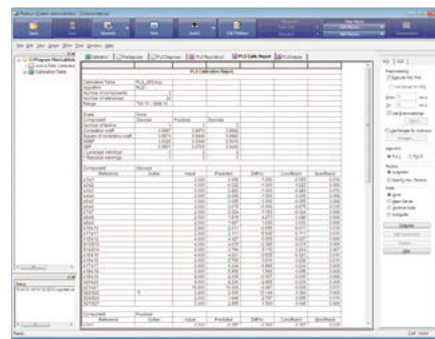


LabSolutions IR

PLS Quantitation program

(P/N 206-74560-91)

PLS (partial least squares) quantitation is a chemometrics method that, like multiple linear regression analysis, is widely used for the simultaneous quantitation of multiple components. The PLS quantitation program incorporates PLS I and PLS II methods. It is possible to display calculation values based on input values. PLS factors are based on "PRESS" values, loading vectors, and score values. Analysis can be performed on the regression equations obtained with the PLS method.

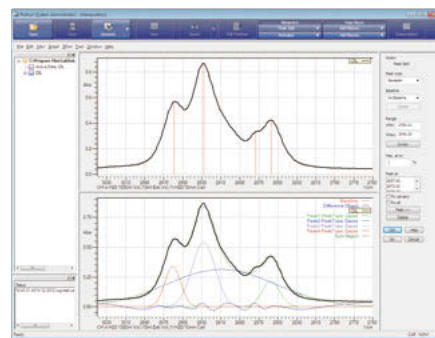


LabSolutions IR

Curve-Fitting (Peak-Splitting) program

(P/N 206-74561-91)

Usually, absorption bands in infrared spectra consist of overlapping peaks. The curve-fitting (peak-splitting) program can be used to separate absorption bands into individual peaks, separate peaks that have been influenced by hydrogen bonding, and identify the peaks of functional groups that are hidden by absorption bands. Six types of curves, such as Gaussian, Lorentzian, and Gaussian+Lorentzian, are available for separation analysis. The curve can be selected in accordance with the form of the peaks in the absorption band. The separated component peaks are displayed together with the resultant spectra, making it possible to accurately evaluate the separation.



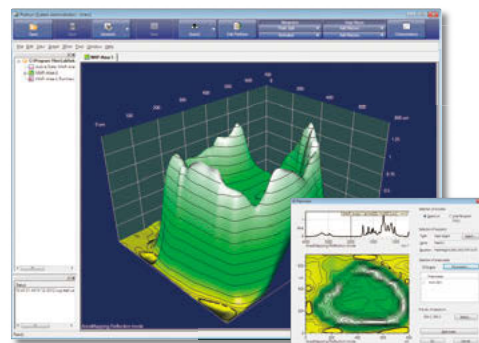
LabSolutions IR

3D processing program

(P/N 206-74563-91)

The 3D processing program offers the following functionality

- ▶ **Changes the method of displaying data**
 - Data can be displayed in bird's eye view (3D), as an intensity distribution or using contour lines, as a spectral overlay, or rotated.
- ▶ **3D data processing**
 - Changes at specific wavenumbers can be isolated.
 - Functions include data extraction, data points thinning, smoothing, zero-baseline, background correction, normalization, log conversion, first- or second-order derivative, and ATR correction.
- ▶ **Creation of 3D data from spectra**
 - Spectra measured at fixed intervals, such as by repeated measurements, can be arranged consecutively to create 3D data.



* The 3D processing program cannot control mapping measurements or AIM-8800 series infrared microscopes.

LabSolutions IR

Macro platform

(P/N 206-74562-91)

The Macro Platform is required to run the customized macro programs created by Shimadzu (for a fee). If, for example, you wish to perform routine work in which certain functions are used

in a pre-determined order, or you wish to run an automatic measurement system in combination with an auto sample changer, please contact your SHIMADZU representative for details.

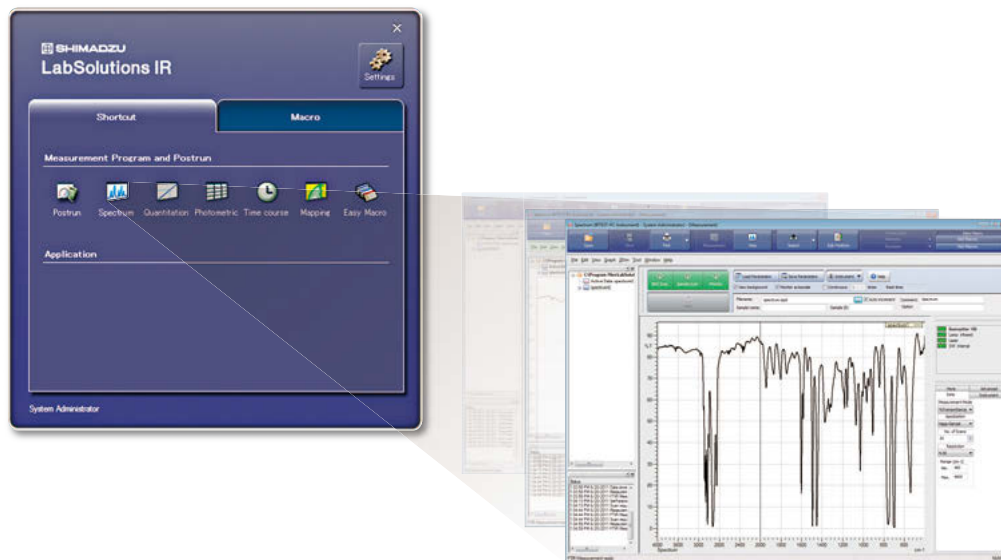
More Benefits of LabSolutions IR

Tailored programs that are easy to run

LabSolutions IR comes with programs tailored to particular FTIR analyses, including postrun analysis, spectrum measurement, and quantitative measurement. These programs are easily accessible from a LabSolutions launcher, which can also be populated with frequently-used Windows applications and simple macro programs.

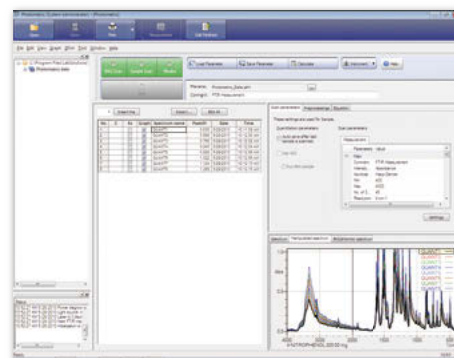
Better operability thanks to a consistent graphical user interface

All postrun analysis programs and measurement programs share a consistent interface in terms of design and operational use, employing a main toolbar, menu, measurement toolbar, tree view, and log window. The same functional steps can be used to operate any of the tailored FTIR analysis programs.



◆ Photometric measurement

The analysis of a spectrum at a particular wavenumber for absorbance, transmittance, peak height, peak area, and peak ratio. These values can be utilized along with various formulae, and to perform a variety of calculations. Threshold values may also be chosen and a pass/fail judgment made on them. These features are useful for calculating saponification, response rate, component ratio, and the like.



◆ Quantitative measurement

A calibration curve is calculated from peak height, peak area, and peak ratio measurements taken from a spectrum of a sample of known concentration. This calibration curve is then used to calculate the concentration of samples of unknown concentration. The calculated concentrations are then inserted into various formulae to perform further calculations. Threshold values can also be chosen and a pass/fail judgment made on them.



Specifications

OS	Microsoft Windows 7 Professional (32 bit / 64 bit)
Instruments	FTIR Infrared Microscope · IRTracer-100 · IRPrestige-21 · IRAffinity series · FTIR-8400 series (OS must be Windows 7 Professional 32 bit.) · AIM-8800
Programs	Postrun analysis, spectrum measurement, quantitative measurement, photometric measurement, time course measurement (option), mapping measurement (option)
Measurement Modes	Spectrum measurement, continuous measurement, atmospheric correction measurement, continuous measurement using ASC, simple measurement
Hardware Monitor	Self-diagnosis function, status monitor
Data Processing Functions	Addition, subtraction, multiplication, division, normalization, baseline correction (zero-baseline correction, 3-point baseline correction, multipoint baseline correction), smoothing, differentiation, X-axis range adjustment, data correction, data points thinning/interpolation, wavenumber-wavelength conversion, X-axis correction, time-temperature conversion, peak detection, point pick, film thickness calculation, data calculation, coincidence, deconvolution, Fourier transformation, Kubelka-Munk conversion, ATR correction, advanced ATR correction, Kramers-Kronig analysis, atmospheric correction, Purity Judgement
Data Processing Functions (Option)	Curve fitting, 3D recalculation, spectrum extraction from 3D data
Search Functions	Spectrum search (based on similarity), peak search, text search, compound search, setting of search conditions, search of user library and commercial library, creation of user library. Libraries containing 12,000 spectra, including those of general organic substances, polymers, pharmaceutical products supplies, inorganic compounds, food additives, and contaminants, are provided.
Quantitative Functions	Multi-point calibration curve method, CLS quantitation method, PLS quantitation method (option), photometric, recalculation function for quantitative and photometric results
Printing Functions	Creation of report template, printing of report template, Easy printing using the view print function
Validation Programs	Validation program that complies with the Japanese, European, Chinese, and United States Pharmacopoeias and with ASTM
GLP/GMP Compliance	Tree-structured audit trail function, recording of operation logs and data logs (history), prohibition of overwriting files with the same file name
Security Functions	Linked with the LabSolutions security functions, authorization setting available for each user group
Macro Program Functions	Easy macro function · Simply creating a list of operational steps executes multiple operations in one go. · Can be run from the desktop Macro platform (option)
Software Options	Time course software, Mapping program, PLS quantitation program, Curve-fitting program, 3D presentation, Macro platform, CLASS-Agent connection kit
File Formats	JCAMP-DX, ASCII, CSV, IRsolution, and HYPER-IR formats can be read and saved.

Computer / Printer

Type	Desktop
Specifications	Provide a computer and printer of a type recommended by Shimadzu. Inquire separately for detailed specifications.



Shimadzu Corporation

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